Semiflexible
Polymer
Elasticity

by

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Certificate:

This is to certify that the thesis entitled "Semiflexible Polymer Elasticity" submitted by Abhijit Ghosh for the award of the degree of Doctor of Philosophy of Jawaharlal Nehru University is his original work. This has not been published or submitted to any other University for any other Degree or Diploma.

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Declaration:

I hereby declare that the work reported in this thesis is entirely original. This thesis is composed independently by me at Raman Research Institute under the supervision of Prof. Joseph Samuel. I further declare that the subject matter presented in this thesis has not previously formed the basis for the award of any degree, diploma, membership, associateship, fellowship or any other similar title of any university or institution.

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Dedicated to

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SOME OF THE WORK DESCRIBED IN THIS THESIS APPEARS IN THE FOLLOWING PAPERS:

[1] **A. Ghosh**, Supurna Sinha, J.A. Dharmadhikari, S. Roy, A.K. Dharmadhikari, J. Samuel, S. Sharma and D. Mathur :

Euler buckling - induced folding and rotation of red blood cells in an optical trap

Phys. Biol **3**, 67-73 (2006); arxiv: physics/0501099.

[2] Joseph Samuel, Supurna Sinha and **Abhijit Ghosh**:

DNA Elasticity: Topology of Self Avoidance

J. Phys.: Condens. Matter **18**, (2006), s253 - s268, arXiv: cond-mat/ 0504189.

[3] **Abhijit Ghosh**, J. Samuel and Supurna Sinha:

Elasticity of Stiff Biopolymers

Phys. Rev. E **76**, 061801 (2007); arXiv: cond-mat/ 0710.1465

(Also selected for the December 15, 2007 issue of Virtual Journal of Biological Physics Research. Link - http://www.vjbio.org)

[4] **Abhijit Ghosh**:

Writhe Distribution of Stiff Biopolymers

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Contents

Preface

This thesis focuses on the statistical physics of semiflexible polymers. There has been a lot of interest in semiflexible polymers in recent years. Flexible polymers have been studied extensively. In case of flexible polymers, consecutive bond segments are totally uncorrelated and a flexible polymer can be modelled as a random walk without any memory; such a model of a flexible polymer is known as the FREELY JOINTED CHAIN (FJC). The polymer remains correlated only over the distance of the bond segment; this is known as the persistence length. The persistence length can be crudely described as the length scale over which the polymer approximately remains straight. When short range interactions between the bond segments are introduced (as in the freely rotating chain/ Kratky Porod model), one talks of the “Kuhn Length” which is the segment length of the equivalent FJC with the same contour length and the same average end-to-end distance. Semiflexible polymers are modelled as a continuous space curve parametrized by an arc length parameter with a unit tangent vector at each point. The length scale over which the tangent-tangent correlation becomes insignificant is known as the persistence length. This model for semiflexible polymers is known as the WORM LIKE CHAIN (WLC). The WLC model is like a random walk with memory.The WLC model has been extended to include twist degrees of freedom as well.

In recent years there has been a lot of interest in the physics of biopolymers like DNA and filamentary proteins like actin. These polymers are essential for many life processes and as cellular components. DNA carries the vital genetic information that need to be accessed during cell division. The elasticity of the cell membrane and its structural stability depends on semiflexible polymers like microtubules and actin filaments present in the cell membrane. The elasticity of these biopolymers is studied via single molecule experiments which probe force-extension relations, torque-twist relations, distribution of end-to-end distance and so on. These experimentally studied phenomena can be nicely modelled by the WLC model.

In chapter 1, we have briefly introduced the essential features of different models of the polymer. We have described briefly the **Freely Jointed Chain (FJC)** model and the **Worm Like Chain Model (WLC)**. We have elucidated the predictions of the **WLC** model with pure bend following Samuel and Sinha. The extension to include twist degrees of freedom to study the elastic properties of a torsionally constrained polymer has been studied following Bouchiat and Mezard. We have briefly alluded to a similar piece of work by Moroz and Nelson.

In chapter 2 we present a statistical mechanical study of stiff polymers, motivated by experiments on actin filaments and the considerable current interest in polymer networks. We have obtained simple, approximate analytical forms for the force-extension relations and compared these with numerical treatments. We have noted the important role of boundary conditions in determining force-extension relations. The theoretical predictions presented here can be tested against single molecule experiments on neurofilaments and cytoskeletal filaments like actin and microtubules. Our work is motivated by the buckling of the cytoskeleton of a cell under compression, a phenomenon of interest to biology. We then extend the above treatment to study the twist elasticity of stiff polymers in the paraxial approximation. We have obtained simple, approximate analytical forms for the writhe distribution at zero applied force. We have also derived simple analytical expressions for the torque-extension relation and the torque-twist relation and discussed buckling of stiff polymers due to the applied torques. We expect our work to initiate experimental efforts in this direction.

In chapter 3 we have described a theoretical treatment of DNA stretching and twisting experiments, in which we have discussed global topological subtleties of self avoiding ribbons and provided an underlying justification for the worm like rod chain (WLRC) model proposed by Bouchiat and Mezard. Some theoretical points regarding the WLRC model are clarified: the "local writhe formula" and the use of an adjustable cutoff parameter to "regularise" the model. Our treatment brings out the precise relation between the worm like chain (WLC), the paraxial worm like chain (PWLC) and the WLRC models. We have described the phenomenon of "topological untwisting" and the resulting collapse of link sectors in the WLC model and note that this leads to a free energy profile *periodic* in the applied link. This periodicity disappears when one takes into account the topology of self avoidance or at large stretch forces (paraxial limit). We note that the difficult nonlocal notion of self avoidance can be replaced (in an approximation) by the simpler local notion of “south avoidance”. This gives an explanation for the efficacy of the approach of Bouchiat and Mezard in explaining the “hat curves” using the WLRC model, which is a south avoiding model. We have proposed a new class of experiments to probe the continuous transition between the periodic and aperiodic behavior of the free energy.

In chapter 4 we have discussed the physics of an optically-driven micromotor of biological origin. A single, live red blood cell, when placed in an optical trap folds into a rod-like shape. If the trapping laser beam is circularly polarized, the folded RBC rotates. A model based on geometric considerations, using the concept of buckling instabilities, captures the folding phenomenon; the rotation of the cell is rationalized using the Poincarè sphere. We predict that (i) at a critical power of the trapping laser beam the RBC shape undergoes large fluctuations and (ii) the torque is proportional to the power of the laser beam. These predictions have been tested experimentally. We have suggested a possible mechanism for emergence of birefringent properties in the RBC in the folded state.

In chapter 5 we have concluded the main body of the thesis with an overview of the work that has been presented in this thesis with some remarks about future directions.